

# One-electron systems in a strong magnetic field

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Using a variational method we study a sequence of the one-electron atomic and molecular-type systems  $H$ ,  $H_2^+$ ,  $H_3^{(2+)}$  and  $H_4^{(3+)}$  in the presence of a homogeneous magnetic field ranging  $B = 0 - 4.414 \times 10^{13} G$ . These systems are taken as a linear configuration aligned with the magnetic lines. For  $H_3^{(2+)}$  the potential energy surface has a minimum for  $B \sim 10^{11} G$  which deepens with growth of the magnetic field strength (*JETP Lett.* **69**, 844 (1999)). For  $B \gtrsim 10^{12} G$  the minimum of the potential energy surface becomes sufficiently deep to have longitudinal vibrational state. We demonstrate that for the (*ppppe*) system the potential energy surface at  $B \gtrsim 4.414 \times 10^{13} G$  develops a minimum, indicating the possible existence of exotic molecular ion  $H_4^{(3+)}$ . It is shown that for almost all accessible magnetic fields  $H_2^+$  is the most bound one-electron system while for magnetic fields  $B \gtrsim 10^{13} G$  the molecular ion  $H_3^{(2+)}$  becomes the most bound.

## I. INTRODUCTION

In the presence of a strong magnetic field the properties of atomic and molecular systems change substantially leading to new unexpected phenomena. It has been a long time since the predictions made by Kadomtsev and Kudryavtsev [1], and Ruderman [2], about the possible existence of unusual chemical compounds in the presence of a strong magnetic field. This phenomenon can be explained by the effective quasi-one-dimensionality of Coulombic systems appearing due to the enormous Lorentz force acting on a system in transverse direction. The transverse size of such systems is governed by the magnetic field and is of the order of the cyclotron radius  $\hat{\rho} \sim B^{-1/2}$  while the longitudinal size remains of atomic (molecular) order shrinking logarithmically  $\sim 1/\log B$  (see, for example, [3]). As a consequence of such quasi-one-dimensionality the electron-nuclei attraction becomes more effective, yielding the possibility of compensating the Coulombic repulsion of nuclei and thus to the possible existence of exotic systems that do not exist without a magnetic field. In particular, the presence of a strong magnetic field can lead to the formation of linear molecules (linear chains) situated along magnetic lines [2,4–6]. Recently, the first quantitative study of the possible existence of the exotic molecular ion  $H_3^{(2+)}$  or, in other words, a bound state in the system of three protons and an electron (*pppe*) was carried out [7]. It turned out that for  $B > 10^{11} G$  the potential energy surface as a function of internuclear distances possesses a minimum, which deepens with magnetic field growth. It provides an evidence that for magnetic fields  $B > 10^{11} G$  such molecular ion can exist [7]. In the present article we extend this study and show that for magnetic fields  $B > 10^{13} G$  another exotic molecular ion  $H_4^{(3+)}$  or bound state in (*ppppe*) can exist.

The aim of this article is to perform a detailed quantitative study and comparison of the one-electron systems  $H$ ,  $H_2^+$ ,  $H_3^{(2+)}$  and  $H_4^{(3+)}$  in strong magnetic field. Our study is limited to an exploration of the ground state only. It is assumed that the Born-Oppenheimer approximation holds, which implies that the positions of protons are kept fixed. We consider the linear molecular configuration for which the protons are aligned with the magnetic field (linear configuration parallel to a magnetic line). This configuration looks optimal from a physical point of view. Spin effects (linear Zeeman effect) are neglected. The magnetic field ranges from 0 up to  $4.414 \times 10^{13} G$ , where non-relativistic considerations hold (for a detailed discussion see, for instance, [6] and references therein). In order to study the stability of the system  $H_3^{(2+)}$ , the longitudinal vibrational modes of the nuclei are considered, while transversal modes (deviation from linearity of the configuration as well as alignment along magnetic line) are not taken into account. The position of the lowest longitudinal vibrational state is estimated.

Our calculations demonstrate that for all studied one-electron systems the binding energy  $E_b = B - E_{total}$ <sup>1</sup> (affinity to keep the electron bound) grows with the increase of the magnetic field strength for  $B = 0 - 4.414 \times 10^{13} G$ . For almost all accessible magnetic fields  $B \lesssim 10^{13} G$  the molecular ion  $H_2^+$  (see the results in [8]) is the most bound one-electron system while for magnetic fields  $B > 10^{13} G$  the molecular ion  $H_3^{(2+)}$  becomes the most bound. Our calculations show as well that for magnetic fields  $B > 10^{13} G$  the potential energy surface of the system (*ppppe*) exhibits the appearance of a minimum indicating the possible formation of such a molecular ion  $H_4^{(3+)}$ . It hints at

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<sup>1</sup>Here  $B$  in  $Ry$  has a meaning of the energy of electron in magnetic field.

a certain hierarchy of the thresholds for the appearance of new one-electron system:  $H_3^{2(+)}$  – at  $B > 10^{11}G$ ,  $H_4^{3(+)}$  – at  $B > 10^{13}G$  etc <sup>2</sup>. If this is so, it is very unlikely that the system  $H_5^{4(+)}$  can appear for magnetic fields existing on the surface of neutron stars. For larger magnetic fields a reliable study requires taking into account relativistic corrections. This is beyond of the scope of this article.

## II. METHOD

The present calculations are carried out in the framework of a variational method using, for each system, a *unique* simple trial function equally applicable to any value of the magnetic field strength. For a successful study a wise choice of trial functions is needed. A constructive criterion for an adequate choice of trial function (see [9]— [14]) is the following: (i) the trial function  $\Psi_t(x)$  should include all symmetry properties of the problem in hand; (ii) if the ground state is studied, the trial function should not vanish inside the domain where the problem is defined; (iii) the potential  $V_t(x) = \frac{\nabla^2 \Psi_t}{\Psi_t}$ , for which the trial function is an exact eigenfunction, should reproduce the original potential behavior near singularities as well as its asymptotic behavior.

Let us first introduce notation (see Fig. 1). We consider identical, infinitely-heavy centers of unit charge situated on the  $z$ -axis. The magnetic field of strength  $B$  is directed along the  $z$  axis,  $\vec{B} = (0, 0, B)$ . Throughout the paper the Rydberg is used as the energy unit. For the other quantities standard atomic units are used.

The potentials corresponding to the systems we study are given by

$$\begin{aligned} V &= -\frac{2}{r} + \frac{B^2 \rho^2}{4}, & H \\ V &= \frac{2}{R} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{B^2 \rho^2}{4}, & H_2^+ \\ V &= \frac{2}{R_1} + \frac{2}{R_2} + \frac{2}{R_1+R_2} - \frac{2}{r_1} - \frac{2}{r_2} - \frac{2}{r_3} + \frac{B^2 \rho^2}{4}, & H_3^{(2+)} \\ V &= \frac{2}{R_1-R_2} + \frac{2}{R_1+R_3} + \frac{2}{R_1+R_4} + \frac{2}{R_2-R_3} + \frac{2}{R_2+R_4} + \frac{2}{R_4-R_3} - \frac{2}{r_1} - \frac{2}{r_2} - \frac{2}{r_3} - \frac{2}{r_4} + \frac{B^2 \rho^2}{4}, & H_4^{(3+)} \end{aligned} \quad (1)$$

where the quantity  $\rho = \sqrt{x^2 + y^2}$  is the distance from the electron to the  $z$ -axis, and the  $r_i$  are the distances from the electron to the  $i$ th center.

## III. TRIAL WAVE FUNCTIONS

A class of trial functions which satisfy the above-mentioned criterion incorporating the basic physical features of Coulomb systems in a magnetic field directed along the  $z$ -axis contains a function

$$\begin{aligned} \psi_0 &= e^{-\varphi(r_1, \dots, r_N, \rho)}, \\ \varphi(r_1, \dots, r_N, \rho) &= \sum_{i=1}^N \alpha_i r_i + \beta B \rho^2 / 4 \end{aligned} \quad (2)$$

as a basic element, where  $\alpha_i$  and  $\beta$  are variational parameters, and  $N$  is the number of centers. This function is nothing but the product of ground-state Coulomb functions and the lowest Landau orbital and is the exact eigenfunction of the potential

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<sup>2</sup>In framework of non-relativistic consideration it can be easily checked that there exist magnetic fields for which a potential energy surface for  $H_5^{4(+)}$  etc can develop a minimum.

$$\begin{aligned}
V_0 &= \frac{\Delta\psi_0}{\psi_0} = [-\nabla^2\varphi + (\nabla\varphi)^2] \\
&= -2\sum_i \alpha_i \frac{1}{r_i} - \beta B + \sum_{i,j} \alpha_i \alpha_j (\hat{n}_i \cdot \hat{n}_j) + \sum_i \alpha_i \beta B \frac{\rho^2}{r_i} + \beta^2 \frac{B^2 \rho^2}{4}, \\
\hat{n}_i \cdot \hat{n}_j &= \frac{1}{r_i r_j} [\rho^2 + (z - z_i)(z - z_j)],
\end{aligned} \tag{3}$$

where  $\hat{n}_i$  is unit vector in  $i$ th direction. This potential reproduces Coulomb-like behavior near the centers and two-dimensional oscillator behavior in the  $(x, y)$  plane at large distances (cf. (1)).

Since the centers are identical the problem possesses permutation symmetry. Hence the ground state trial function must be permutationally-symmetric with respect to permutation of positions of the centers,  $r_i \leftrightarrow r_j$ .

One of the simplest functions satisfying the above-mentioned criterion is the function (2) itself with the same  $\alpha$ 's (those can be placed equal to  $\alpha_1$ ):

$$\Psi_1 = e^{-\alpha_1 (\sum_{i=1}^N r_i) - \beta_1 B \rho^2 / 4}, \tag{4}$$

where  $\alpha_1, \beta_1$  are variational parameters. Actually, this function is a Heitler-London type function multiplied by the lowest Landau orbital. If the internuclear distances are taken as parameters, it has in total  $(N + 1)$  variational parameters. It is quite natural from a physical viewpoint to assume that this function gives a description of the system near the equilibrium position. The potential  $V_1(x) = \frac{\nabla^2 \Psi_1}{\Psi_1}$ , corresponding to this function is:

$$V_1 = N\alpha_1^2 - B\beta_1 - 2\alpha_1 \sum_{i=1}^N \left( \frac{1}{r_i} \right) + \frac{\beta_1^2 B^2 \rho^2}{4} + 2\alpha_1^2 \sum_{i < j} \hat{n}_i \cdot \hat{n}_j + \alpha_1 \beta_1 B \rho^2 \sum_{i=1}^N \left( \frac{1}{r_i} \right), \tag{5}$$

(cf. (3)).

Another possible trial function is a permutationally-symmetric linear superposition of the functions (2) in which all  $\alpha$ 's are placed to be equal to zero except one, which is denoted  $\alpha_2$

$$\Psi_2 = \left( \sum_{i=1}^N e^{-\alpha_2 r_i} \right) e^{-\beta_2 B \rho^2 / 4}. \tag{6}$$

Here  $\alpha_2, \beta_2$  are variational parameters. This function is a Hund-Mulliken type function multiplied by the lowest Landau orbital. One can assume that when all internuclear distances are sufficiently large this function dominates, giving an essential contribution. Thus, it describes an interaction of the hydrogen atom with  $(N - 1)$  charged centers. This function can also describe a possible decay mode of the studied system to the hydrogen atom and  $(N - 1)$  protons. As in Eq.(4), the trial function (6) is characterized by  $(N + 1)$  variational parameters.

Another trial function describes a possible decay mode  $H_N^{((N-1)+)} \rightarrow H_2^+ + (N - 2)p$ ,  $N \geq 3$ , and is a permutationally-symmetric linear superposition of the functions (2) with all  $\alpha$ 's are equal to zero except two, which are taken to be equal and denoted as  $\alpha_3$ :

$$\Psi_3 = \left( \sum_{i < j} e^{-\alpha_3 (r_i + r_j)} \right) e^{-\beta_3 B \rho^2 / 4}, \tag{7}$$

where  $\alpha_3, \beta_3$  are variational parameters. It seems that the function (7) gives the dominant contribution to the large internuclear distances when the distance between two neighboring centers is kept fixed. It can be true for magnetic fields  $B < 10^{13} G$ , where the system with the lowest total energy is  $H_2^+$ . Eq.(7) also depends on  $(N + 1)$  variational parameters.

Finally, for magnetic fields  $B > 10^{11} G$  where the exotic state  $H_3^{(2+)}$  begins to appear we also introduce a trial function of the form

$$\Psi_4 = \left( \sum_{i < j < k} e^{-\alpha_4 (r_i + r_j + r_k)} \right) e^{-\beta_4 B \rho^2 / 4}. \tag{8}$$

where again  $\alpha_4$  and  $\beta_4$  are variational parameters. This function depends on  $N + 1$  variational parameters.

In order to incorporate in a single trial function the behavior of the system both near equilibrium and at large distances, we use an appropriate interpolation of the trial functions (4), (6), (7) and (8). There are several natural types of such interpolations:

(i) Total non-linear superposition of the form:

$$\Psi_{5-nls} = \left( \sum_{\{\alpha'_1, \dots, \alpha'_N\}} e^{-\alpha'_1 r_1 - \alpha'_2 r_2 - \dots - \alpha'_N r_N} \right) e^{-\beta' B \rho^2 / 4} \quad (9)$$

where  $\alpha'_1, \dots, \alpha'_N$  and  $\beta'$  are variational parameters, and the sum is over all permutations of the parameters  $\{\alpha'_1, \dots, \alpha'_N\}$ . The function (9) is an  $N$ -center modification of the Guillemin-Zener type function used for the description of the molecular ion  $H_2^+$  in a magnetic field (see Eq.(2.5) in [8]). If all parameters coincide  $\alpha'_i = \alpha_1$ ,  $i = 1 \dots N$ , the function (9) reduces to the Heitler-London type function (4). If the only parameter is non-zero, say  $\alpha'_1 = \alpha_2$ , this function reduces to the Hund-Mulliken type wave function (6), if two parameters are non-zero, and equal, say,  $\alpha'_1 = \alpha'_2 = \alpha_3$  it reduces to the trial function (7), and if three parameters are non-zero,  $\alpha'_1 = \alpha'_2 = \alpha'_3 = \alpha_4$  it reduces to (8). In general, there are  $2N$  variational parameters (including the internuclear distances as parameters) characterizing the trial function (9).

(ii) Partial non-linear superpositions:

these are special cases of (9) when two or more parameters are equal. For instance, for  $N = 3$   $\alpha'_1 = \alpha'_2 \neq \alpha'_3$  :

$$\Psi_{6-nls-p} = \left( e^{-\alpha'_1(r_1+r_2)-\alpha'_3 r_3} + e^{-\alpha'_1(r_1+r_3)-\alpha'_3 r_2} + e^{-\alpha'_1(r_2+r_3)-\alpha'_3 r_1} \right) e^{-\beta' B \rho^2 / 4}, \quad (10)$$

This function can be considered as a non-linear interpolation between Eqs. (6) and (7) for the  $H_3^{(2+)}$  ion.

(iii) Linear superposition of Eqs.(4), (6), (7), (8)

$$\Psi_{7-ls} = A_1 \Psi_1 + A_2 \Psi_2 + A_3 \Psi_3 + A_4 \Psi_4, \quad (11)$$

where  $A_1, A_2, A_3, A_4$  are taken as extra variational parameters. It should be mentioned that in general  $\Psi_{1,2,3,4}$  are not orthogonal and thus the parameters  $A_{1,2,3,4}$  do not have a meaning of the weight factors.

So, each of the above interpolations has a certain physical meaning describing different physical situations. In order to make up a rich description of the systems one can take a linear superposition of all previously mentioned functions with factors in front of them, those are treated as extra variational parameters. In this work we use only some particular cases of this general interpolation procedure (see below for details).

The minimization procedure is carried out using the standard minimization package MINUIT from CERN-LIB. All integrals are calculated with relative accuracy  $\leq 10^{-8}$ . We use the integration routine D01FCF from NAG-LIB.

## IV. RESULTS

The results are summarized in Table V. In general, a common feature of the energy dependences for the hydrogen atom  $H$  and molecular ions  $H_2^+$  and  $H_3^{(2+)}$  are characterized by the growth of the binding energy, as well as a decrease of the equilibrium distances ( $R$  for  $H_2^+$ , and  $R_1 + R_2$  for  $H_3^{(2+)}$ ) with increase of magnetic field strengths<sup>3</sup>. It seems reasonable to conjecture that this behavior persists for magnetic fields  $B > 4.414 \times 10^{13} G$  for which a non-relativistic treatment is no longer applicable.

In Table V  $L$  is the “natural” size of the system which is determined by the internuclear distances. For  $H_3^{(2+)}$ , the energy of the lowest vibrational state is defined as  $\delta E = \frac{1}{2} \hbar \omega_+ + \frac{1}{2} \hbar \omega_-$  (with principal axes:  $\mathcal{R}_+ = R_1 + R_2$ ,  $\mathcal{R}_- = R_2 - R_1$ , see Fig. 1). One should emphasize that with a magnetic field growth all studied systems become more and more compact, and also for both  $H_2^+$  and  $H_3^{(2+)}$  the energy of the lowest vibrational state increases.

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<sup>3</sup>It is known that in the limit of large magnetic fields the binding energy of electron in  $H$ ,  $H_2^+$ ,  $H_n$  systems as well as in heavy atoms behaves  $\propto (\log B)^2$  and the equilibrium distances  $\propto (\log B)^{-1}$  (see, for instance, [1,2,4,15] and discussion therein). Similar estimates should hold for other one-electron linear systems.

### A. $H$ -Atom

For the ground state of the  $H$ -atom we use the trial function of the form (2) at  $N = 1$  (see [13]— [14])

$$\psi_H = e^{-\alpha r - \beta B \rho^2/4},$$

where  $\alpha$  and  $\beta$  are variational parameters. A comparison with the results obtained by Lai et al [4] shows that this simple trial function gives a relative accuracy  $10^{-4}$  in energy for magnetic fields  $B = 0 - 4.414 \times 10^{13} G$ . The binding energy for this system increases with magnetic field growth and the longitudinal size reduces drastically from  $1.5 \text{ a.u.}$  at  $B = 0$  to  $0.242 \text{ a.u.}$  at  $B = 4.414 \times 10^{13} G$ . The total energy for the  $H$ -atom is larger than the total energy for  $H_2^+$  for all studied magnetic fields, as well as larger than the total energies for  $H_3^{(2+)}$  and for  $H_4^{(3+)}$  for  $B \gtrsim 10^{11} G$  and  $B \gtrsim 4.414 \times 10^{13} G$ , respectively (see Table I). So, the  $H$ -atom is a least bound one-electron system among  $H_2^+$ ,  $H_3^{(2+)}$  and  $H_4^{(3+)}$ .

### B. $H_2^+$ molecular ion

For this system a linear superposition of trial functions (4), (6) and (9) for  $N = 2$  is used for present variational calculation (cf. [8]). In total there are ten variational parameters and the present calculation provides the most accurate ground state total energy for  $B \gtrsim 10^9 G$ . The ground state corresponds to the positive parity state  $1\sigma_u$ . For magnetic fields in the region  $B = 0 - 10^{13} G$  this system is characterized by the lowest total energy among the one-electron systems we consider, being the most stable. The binding energy increases (and the equilibrium distance  $R$  decreases) with the increase of the magnetic field. It is worth noting that the longitudinal localization length of the electron  $\langle |z| \rangle$  is larger than the “natural” size of the system  $L = R$  for magnetic fields  $B > 0$ . The energy of the lowest longitudinal vibrational level is estimated using a harmonic approximation of the bottom of the potential energy curve. The position of the lowest vibrational state in comparison with the Born-Oppenheimer minimum of the total energy grows steadily from  $\delta E = 0.01 Ry$  at  $B = 0$  to  $\delta E = 1.23 Ry$  for  $B = 4.414 \times 10^{13} G$ , respectively.

### C. $H_3^{(2+)}$ molecular ion

For this exotic system  $H_3^{(2+)}$  theoretical evidence was provided of its existence for magnetic fields  $B > 10^{11} G$  [7]. For the present variational calculations we use a linear superposition of trial functions (4), (6), (7) and (9) for  $N = 3$ . We have in total fourteen variational parameters. As in the case of  $H_2^+$  the binding energy increases, and the natural size of the system  $L = R_1 + R_2$  decreases, as the magnetic field grows. In contrast to the  $H_2^+$  ion, the longitudinal localization length of the electron  $\langle |z| \rangle$  is smaller than the natural size of the system. In this case the electronic cloud mainly surrounds the central proton. The potential energy surface on the plane  $(R_1, R_2)$  exhibits a well-pronounced minimum at  $R_1 = R_2$  starting from  $B \sim 10^{11} G$ . The energy of the lowest longitudinal vibrational state is calculated using a harmonic approximation around the minimum along the principal axes  $\mathcal{R}_+ = R_1 + R_2$ ,  $\mathcal{R}_- = R_2 - R_1$  in the plane  $(R_1, R_2)$ . Our results show that for  $B = 10^{11} G$  the energy of the lowest longitudinal vibrational state in harmonic approximation  $\delta E = 0.189 Ry$  lies much above the top of the barrier  $\Delta E = 0.054 Ry$ . However, the situation changes with growth of magnetic field. For  $B \gtrsim 10^{12} G$  the potential well becomes sufficiently deep to keep the lowest vibrational state inside of the well (see Table I). For  $B = 10^{11} - 10^{13} G$  the system  $H_3^{(2+)}$  is unstable towards a decay to  $H_2^+ + p$ . With the growth of magnetic field the total energy of  $H_3^{(2+)}$  becomes lower than the total energy for  $H_2^+$ . This happens at  $B \approx 4.414 \times 10^{13} G$  and it means that for  $B \gtrsim 4.414 \times 10^{13} G$  the exotic molecular ion  $H_3^{(2+)}$  becomes the most bound one-electron system.

### D. $H_4^{(3+)}$ molecular ion

To study this system we use a superposition of the trial functions (4), (6), (7) and (8) for  $N = 4$  in total with fifteen variational parameters. A symmetry argument implies that the minimum, if it exists, should correspond to the configuration  $R_3 = R_2$  and  $R_4 = R_1$  (see Fig. 1). The results show that for magnetic fields  $B \lesssim 10^{13} G$  the potential energy surface in the plane  $(R_1, R_2)$  do not exhibit any minimum. The first indication to a possible existence of the minimum comes at  $B = 10^{13}$  and for  $B = 4.414 \times 10^{13} G$  the potential energy surface indicates the appearance of a well-pronounced minimum of depth  $\Delta E = 0.4 Ry$  at  $R_1 = 0.225$  and  $R_2 = 0.058$ . The longitudinal localization length

of the electron  $\langle |z| \rangle$  is smaller than the natural size of the system  $L = 2R_1$  similarly to what takes place for  $H_3^{(2+)}$ . The electronic cloud surrounds mainly the two central protons. It is important to stress that the total energy for this system is smaller than the total energy of the  $H$  atom but is larger than the total energy for  $H_2^+$  and  $H_3^{(2+)}$  at  $B = 4.414 \times 10^{13} G$ .

## V. CONCLUSIONS

In the presence of a strong magnetic field the formation of exotic chemical compounds can occur. In particular, in present article we demonstrate that in addition to the  $H$ -atom and the  $H_2^+$  molecular ion two more one-electron systems  $H_3^{(2+)}$  and  $H_4^{(3+)}$  can exist those do not exist without a magnetic field. The results of our consideration show an appearance of a minimum in the potential energy surfaces for the systems ( $pppe$ ) and ( $ppppe$ ) for magnetic fields  $B > 10^{11} G$  and at  $B = 4.414 \times 10^{13} G$ , respectively, indicating the formation of the exotic ions  $H_3^{(2+)}$  and  $H_4^{(3+)}$ . Among these systems the molecular ion  $H_2^+$  possesses the lowest total energy in the region  $B \lesssim 10^{13} G$  being the most stable towards a fission of proton(s) or an electron. The ion  $H_3^{(2+)}$  can decay to  $H_2^+ + p$  but not to  $H + p + p$ . However, for magnetic fields  $B \gtrsim 4.414 \times 10^{13} G$  the ion  $H_3^{(2+)}$  becomes the most stable one-electron system possessing the lowest total energy. Our estimates show that the lowest longitudinal vibrational state of  $H_3^{(2+)}$  can also exist for magnetic fields  $B \geq 10^{12} G$ .

For a magnetic field  $B \simeq 4.414 \times 10^{13} G$ , where we assume that a non-relativistic treatment is still valid, the exotic molecular ion  $H_4^{(3+)}$  can exist. This ion is unstable towards a decay to  $H_2^+ + p + p$  and  $H_3^{(2+) + p}$ , however having no decay mode  $H + p + p + p$ . A further study of this system beyond the non-relativistic treatment is needed for reliable evidence of its existence.

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FIG. 1. One-electron systems in a magnetic field  $B$  – explanation of the notations used. (a)  $H$ -atom, (b)  $H_2^+$ , (c)  $H_3^{(2+)}$ , (d)  $H_4^{(3+)}$ . The positions of charged centers are marked by bullets.

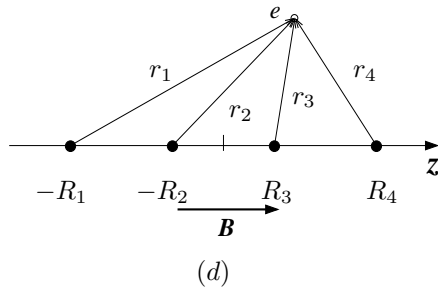
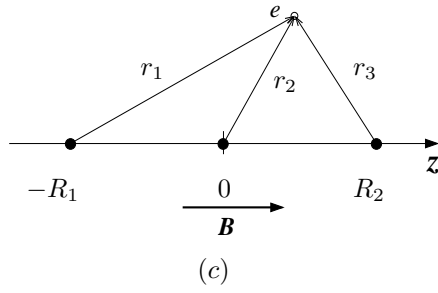
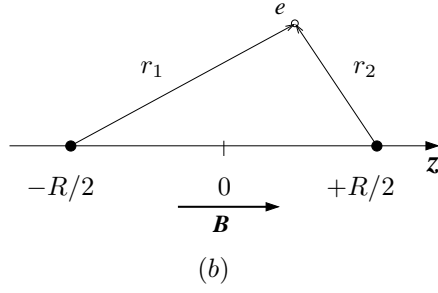
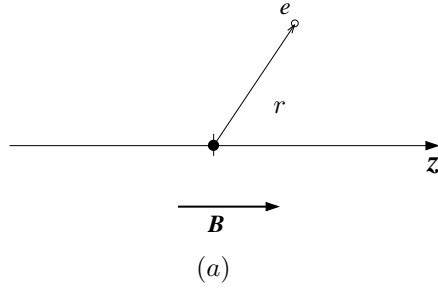
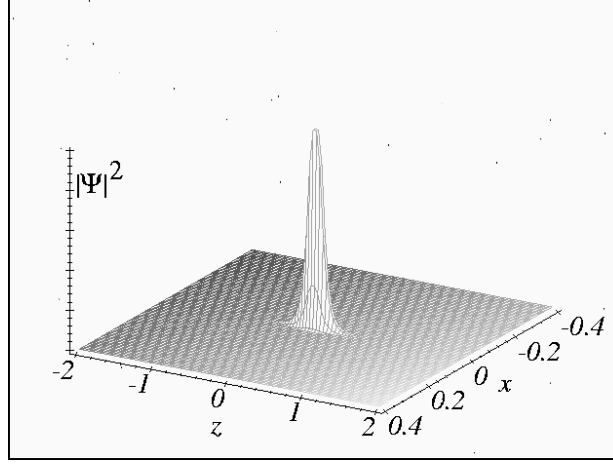
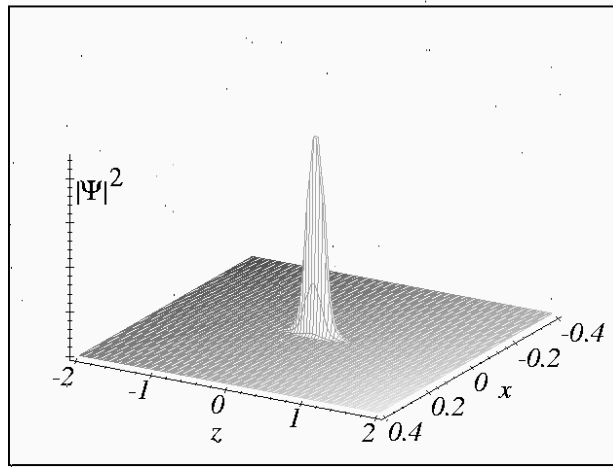




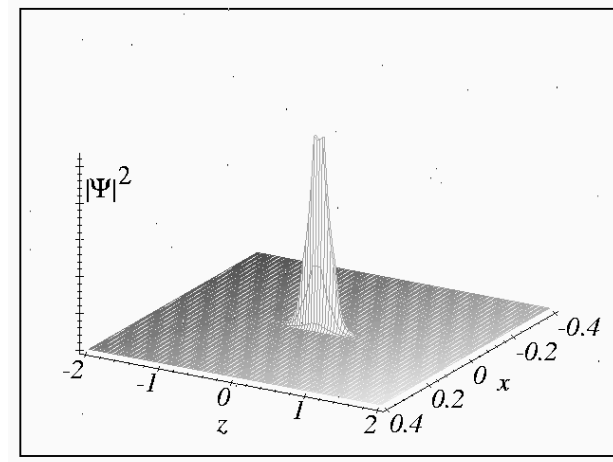
FIG. 2. Electronic probability density for (a)  $H_2^+$ , (b)  $H_3^{(2+)}$  and (c)  $H_4^{(3+)}$  for  $B = 4.414 \times 10^{13} G$ . Normalization of  $|\Psi|^2$  is not fixed.



(a)

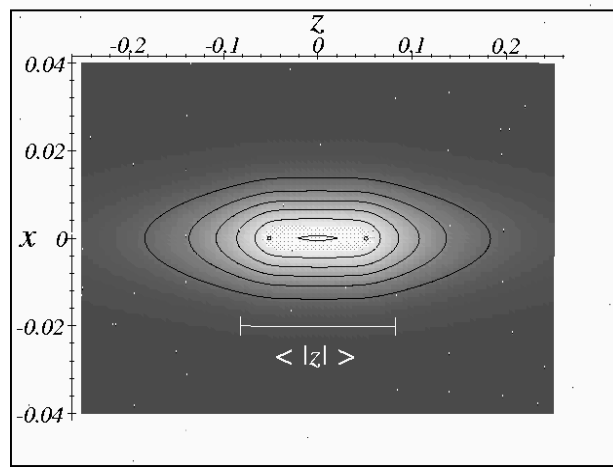


(b)

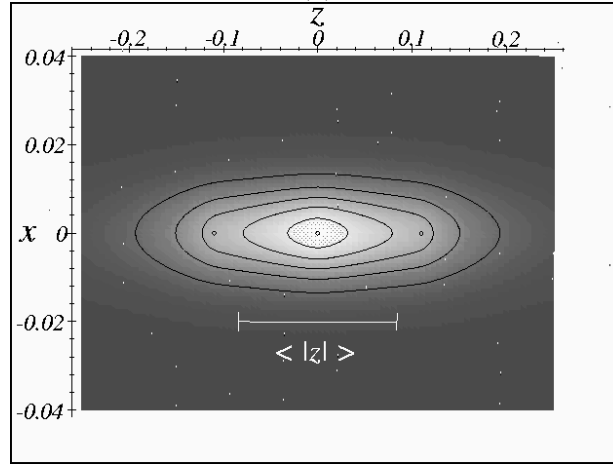


(c)

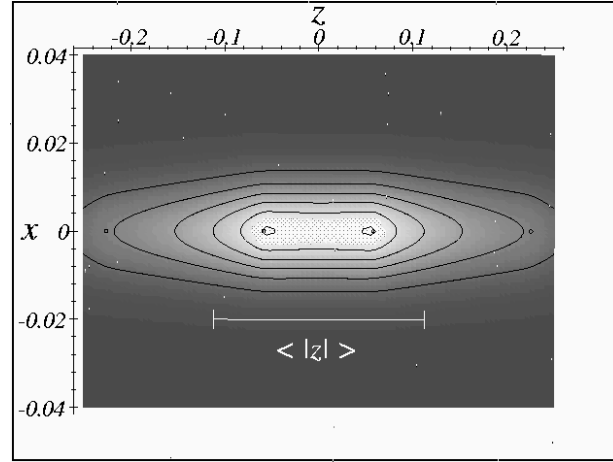
FIG. 3. Electronic probability density contours for (a)  $H_2^+$ , (b)  $H_3^{(2+)}$  and (c)  $H_4^{(3+)}$  for  $B = 4.414 \times 10^{13}$  G. The position of the centers is indicated by small circles. The longitudinal localization length of the electron  $\langle |z| \rangle$  is displayed.



(a)



(b)



(c)

TABLE I. Variational results for the one-electron systems  $H$ ,  $H_2^+$ ,  $H_3^{(2+)}$  and  $H_4^{(3+)}$  in a strong magnetic field for total energy  $E$ , natural size of the system  $L$ , longitudinal electron localization length  $\langle|z|\rangle$ , longitudinal vibrational energy  $\delta E$  measured from the bottom of the well, and the height of the barrier  $\Delta E$  (see text for further explanations). Results in parenthesis are taken from \* Lai et al. [4], \*\* Lai et al. [5], † Wind [16], ‡ Wille [17], †† Kravchenko and Liberman [18], ° [8], °° [7] .

$B$ (Gauss)		$H$	$H_2^+$	$H_3^{(2+)}$	$H_4^{(3+)}$
0	$E$	-1.000	-1.20525°	—	—
		—	(-1.205268†)	—	—
	$L$	—	1.997	—	—
		—	(2.000†)	—	—
	$\langle z \rangle$	1.50	1.704	—	—
	$\delta E$	—	0.0107	—	—
		—	(0.0106 ††)	—	—
	$\Delta E$	—	—	—	—
$10^{11}$	$E$	36.996	35.036°	36.429°°	—
		(36.929*)	(35.043‡)	—	—
	$L$	—	0.593	1.606	—
		—	(0.593‡)	—	—
	$\langle z \rangle$	0.685	0.624	0.864	—
	$\delta E$	—	0.084	0.189	—
		—	(0.074 **)	—	—
	$\Delta E$	—	—	0.054	—
$10^{12}$	$E$	413.94	408.30°	410.296°°	—
		(413.57*)	(408.56‡)	—	—
	$L$	—	0.283	0.692	—
		—	(0.278‡)	—	—
	$\langle z \rangle$	0.441	0.348	0.438	—
	$\delta E$	—	0.259	1.033	—
		—	(0.243 **)	—	—
	$\Delta E$	—	—	0.833	—
$10^{13}$	$E$	4232.6	4218.665°	4220.090°°	—
		(4231.6*)	(4218.674*)	—	—
	$L$	—	0.147	0.330	—
		—	(0.15*)	—	—
	$\langle z \rangle$	0.301	0.214	0.242	—
	$\delta E$	—	0.714	2.406	—
		—	(0.625 **)	—	—
	$\Delta E$	—	—	3.58	—
$4.414 \times 10^{13}$	$E$	18747.4	18724.501	18723.88	18735.70
	$L$	—	0.102	0.220	0.450
	$\langle z \rangle$	0.242	0.164	0.168	0.224
	$\delta E$	—	1.233	4.27	—
	$\Delta E$	—	—	6.5	0.4